Configuration mixing of energy density functionals around ^{32}Mg

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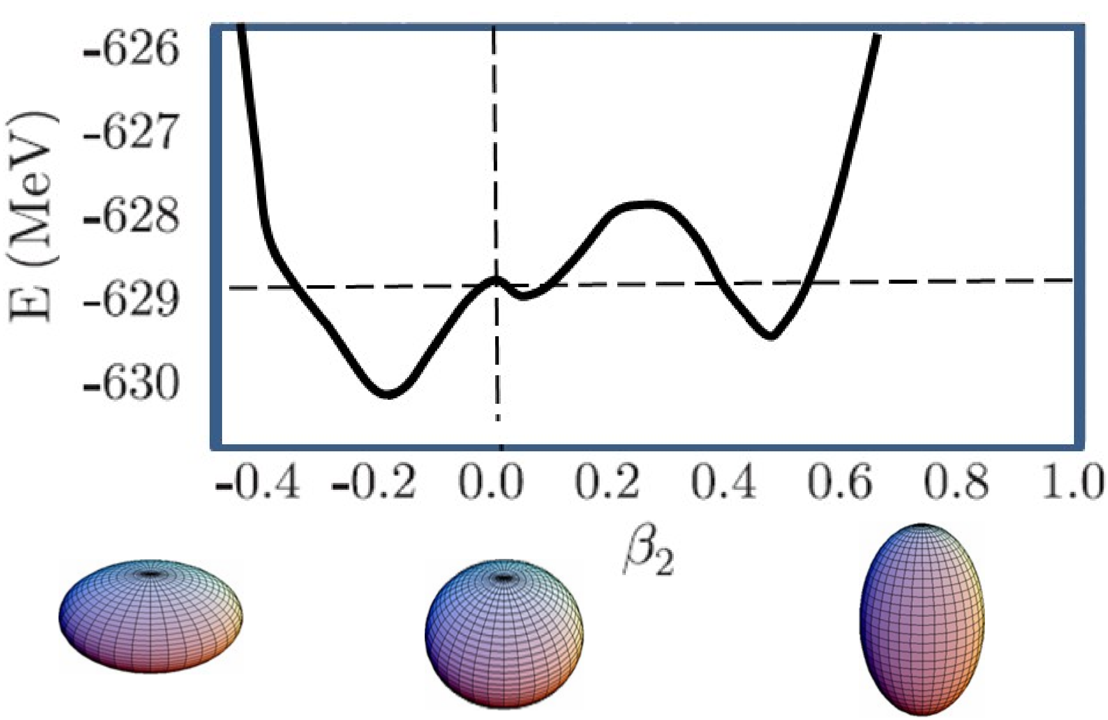
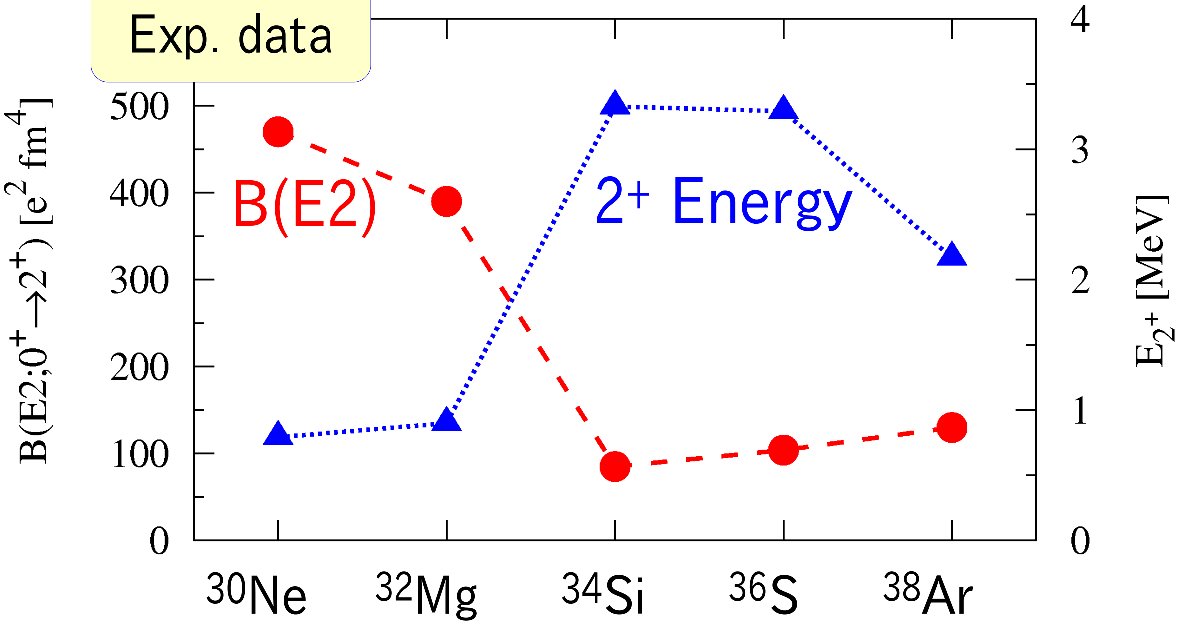


- Introduction
- Configuration mixing
- Problems
- Regularization
- Results
- Outlook

Introduction

- Neutron-rich nuclei around N=20

Exp. data



Thibault et al., PRC12(1975)644
Motobayashi et al., PLB346(1995)9
Yanagisawa et al., PLB566(2003)84
Neyens et al., PRL94(2005)022501

^{32}Mg: Deformed ?

- Mean-field calculations

  → Spherical ground state

Terasaki et al., NPA621(1997)706
Reinhard et al., PRC60(1999)014316

Model beyond mean field …

Configuration mixing

1. Constraint HFB for each deformation

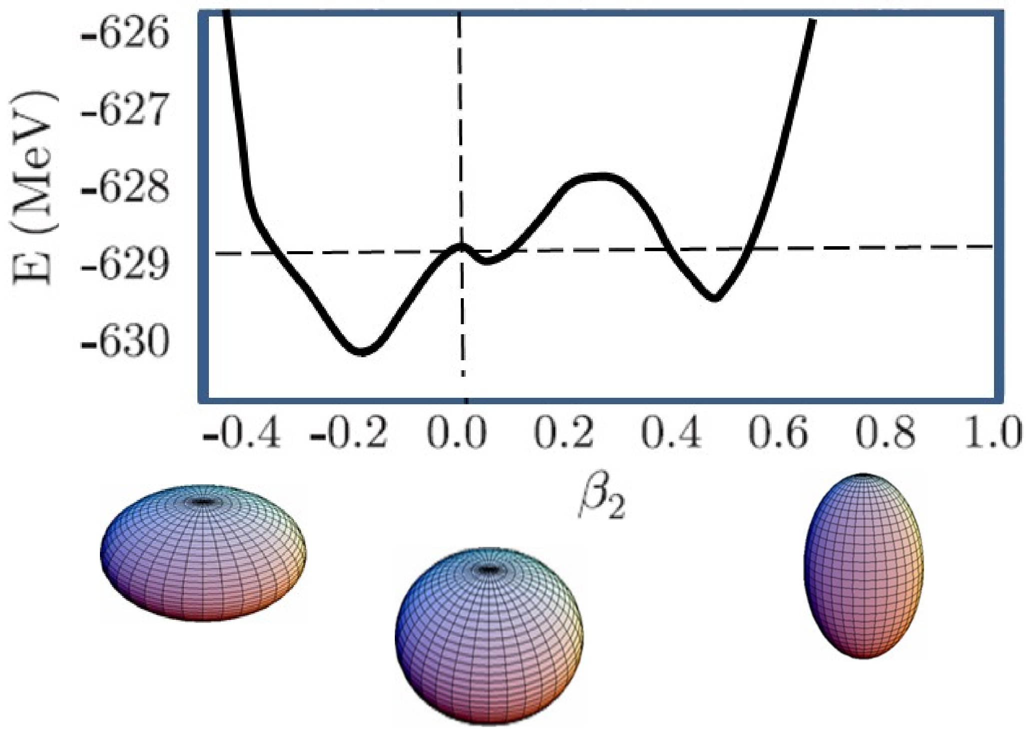
Bender et al., RMP75(2003)121

$$\delta(\mathcal{E} - \lambda_N \langle N \rangle - \lambda_Z \langle Z \rangle - \lambda_Q \langle Q \rangle) = 0$$

$\mathcal{E}$: Skyrme energy density functional

Obtained mean-field states

- Not eigenstate of particle number
- Break rotational symmetry



Restore these symmetries

Projection

Configuration mixing

Valor et al., NPA671(2000)145
Rodriguez-Guzman et al., NPA709(2002)201
Bender et al., PRC74(2006)024312
Bender and Heenen, PRC78(2008)024309

1. Constraint HFB for each deformation

$$\delta(\mathcal{E} - \lambda_N \langle N \rangle - \lambda_Z \langle Z \rangle - \lambda_Q \langle Q \rangle) = 0$$

2. Projection on N, Z, J

$$|JMNZq\rangle = \frac{1}{C_N} \hat{P}^J_{MK} \hat{P}^N \hat{P}^Z |q\rangle$$

$$(q \longrightarrow \beta_2)$$

$$\hat{P}^N = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{i\phi(\hat{N}-N)}$$

$$\hat{P}^J_{MK} = \frac{2J+1}{8\pi^2} \int d\Omega \, \mathcal{D}^{J*}_{MK}(\Omega) R(\Omega)$$

3. Calculate matrix elements

$$\mathcal{H}^J_{qq'} = \langle JMq|H|JMq'\rangle, \quad \mathcal{N}^J_{qq'} = \langle JMq|JMq'\rangle$$

4. Solve the Hill-Wheeler equation

$$\sum_{q'} \left(\mathcal{H}^J_{qq'} - E^J_k \mathcal{N}^J_{qq'}\right) f^J_k(q') = 0$$

$$|JMk\rangle = \sum_q f^J_k(q) |JMq\rangle$$

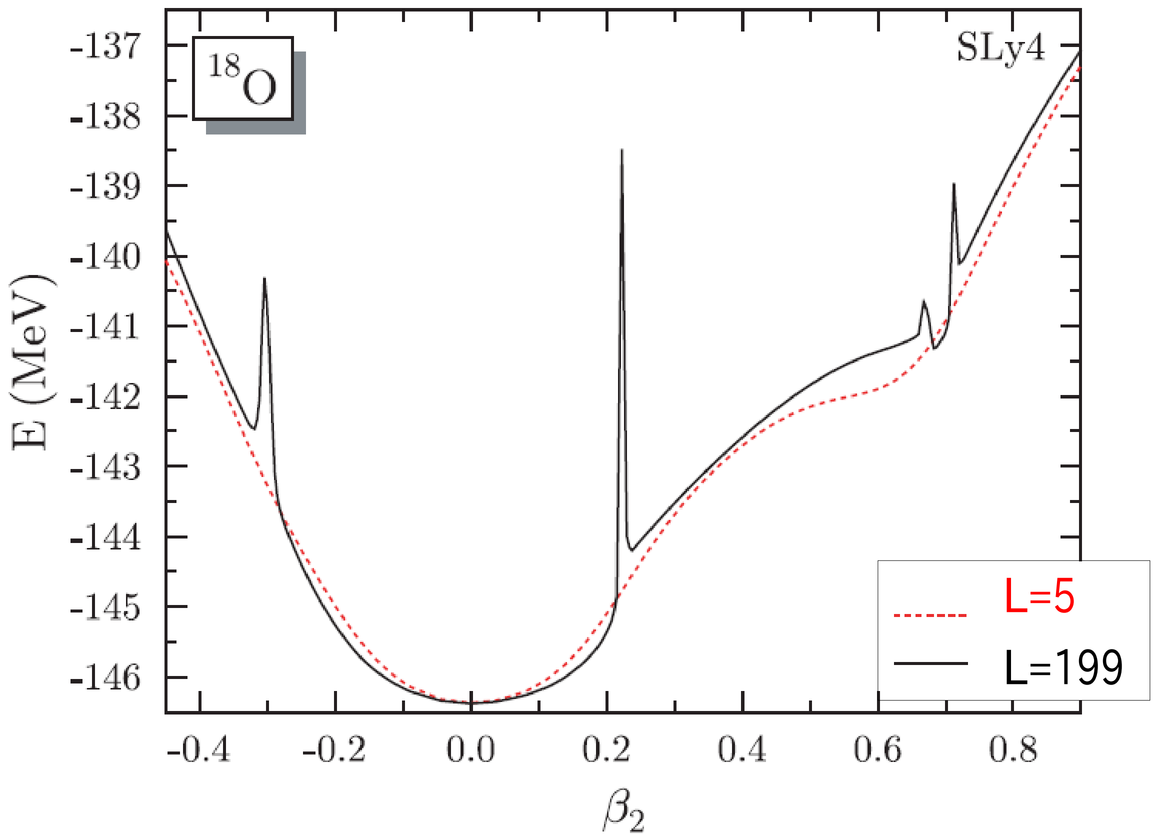
$\Rightarrow$ Collective states

Problems

- Visible in particle-number-projected energy

  Worst example: ^{18}O

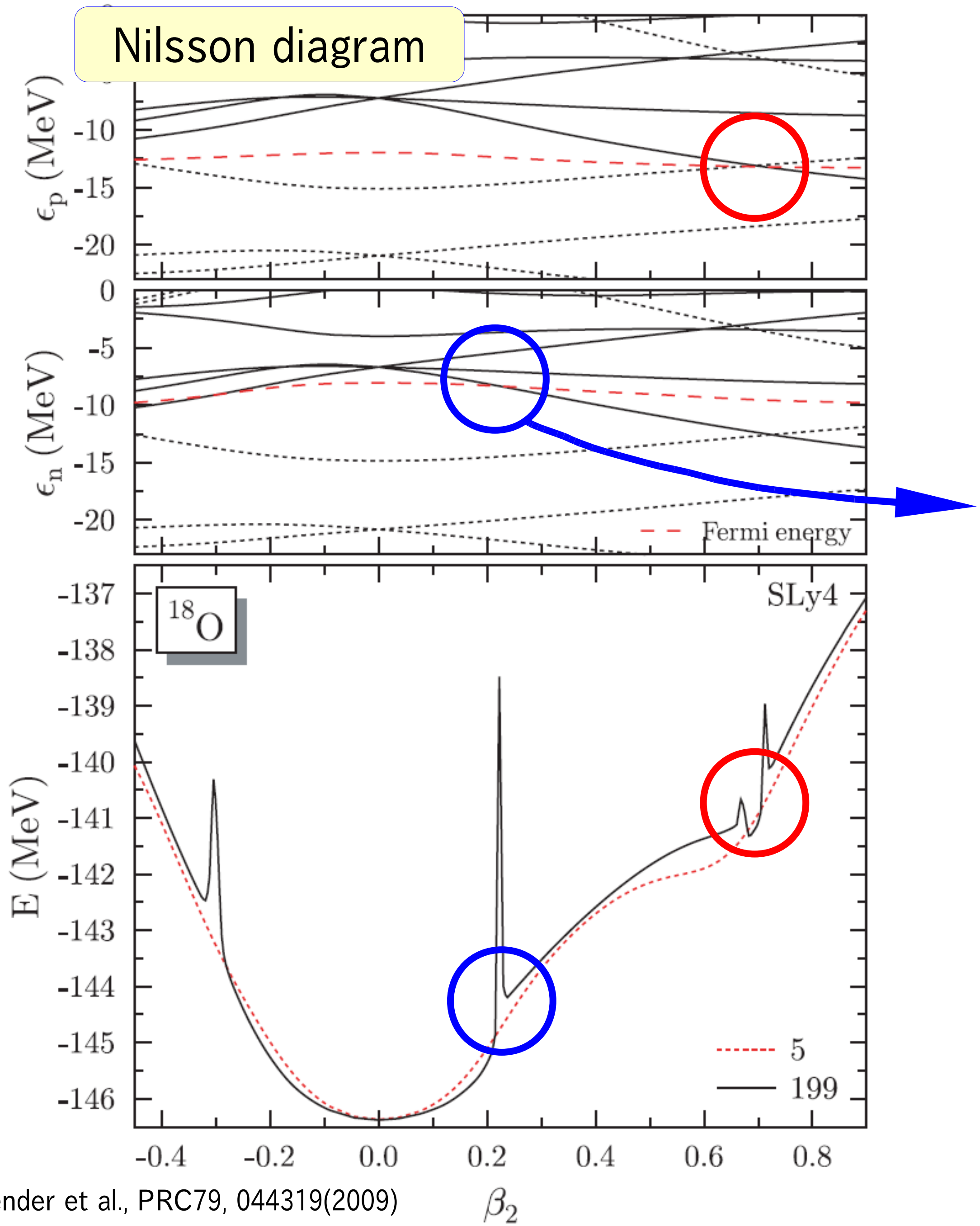
$$E(\beta) = \langle \Phi_N(\beta)|H|\Phi_N(\beta)\rangle$$



$$\begin{aligned} |\Phi_N\rangle &= \frac{1}{\mathcal{N}} P^{N_0}|q\rangle \\ &= \frac{1}{\mathcal{N}} \frac{1}{\pi} \int_0^\pi d\phi\, e^{i\phi(\hat{N}-N_0)}|q\rangle \\ &= \frac{1}{\mathcal{N}} \frac{1}{L} \sum_{\ell=1}^{L} e^{\frac{i\pi(\ell-1)(\hat{N}-N_0)}{L}}|q\rangle \end{aligned}$$

Bender et al., PRC79, 044319(2009)

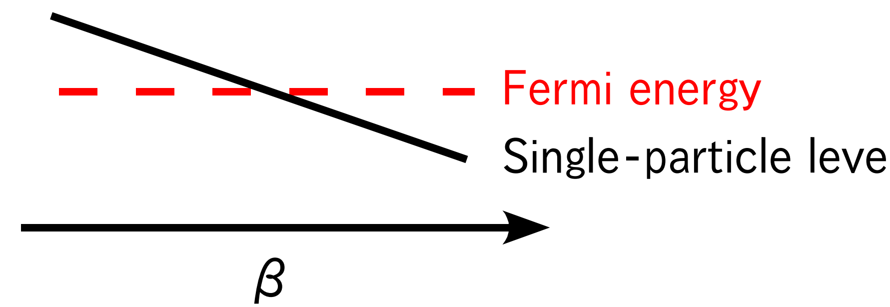
Problems



Bender et al., PRC79, 044319(2009)

Divergence

Crossing



Anguiano et al., NPA696(2001)467

Lacroix et al., PRC79(2009)044318
Bender et al., PRC79(2009)044319
Duguet et al., PRC79(2009)044320

Regularization

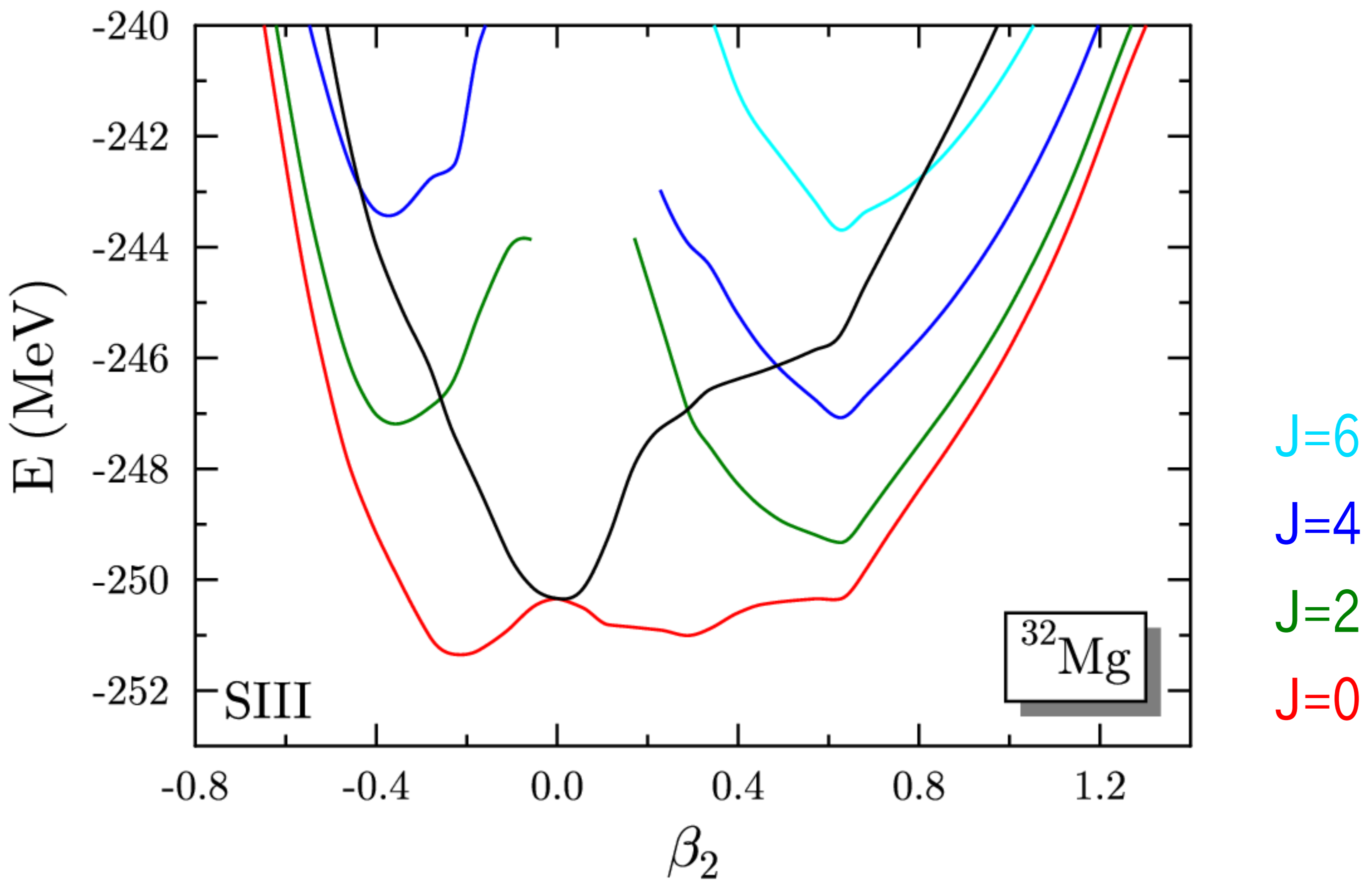
Lacroix et al., PRC79(2009)044318
Bender et al., PRC79(2009)044319
Duguet et al., PRC79(2009)044320

- Divergence should cancel out if $V_{ph} = V_{pp}$
  - ~~Use $V_{ph} = V_{pp}$~~
  - Regularization
    1. Pick up terms that would cancel out if $V_{ph} = V_{pp}$
    2. Remove these contribution from energy functionals

$\Rightarrow$ Divergence will disappear from functionals

Results

Particle-number and J-projected potential energy

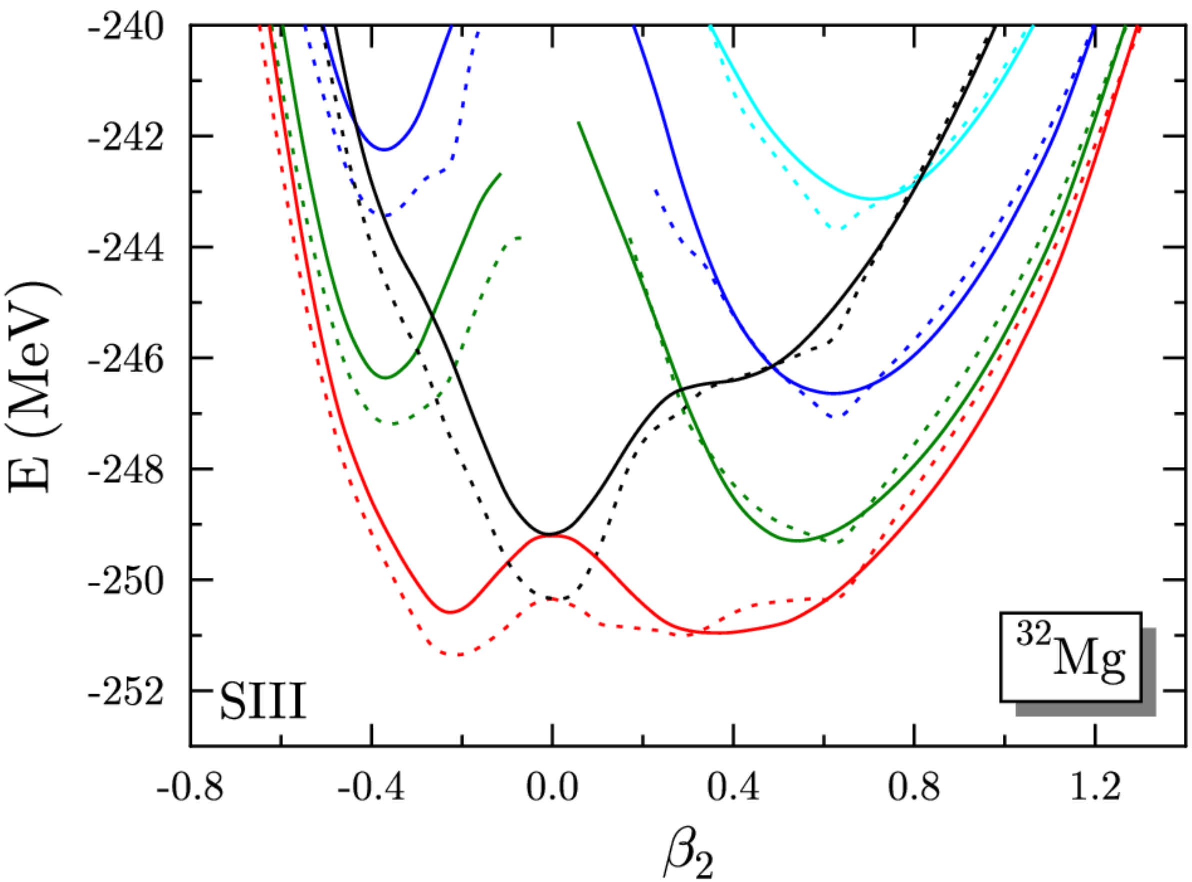


- SIII Skyrme interaction
- Volume type delta-pairing

  Pairing strength: 3 point formula of ^{30}Mg, ^{31}Mg, ^{32}Mg binding energies

Results

Particle-number and J-projected potential energy



- Smoother
- A few MeV correction

  << Binding energy

  ∼ Excitation energy

J=6

J=4

J=2

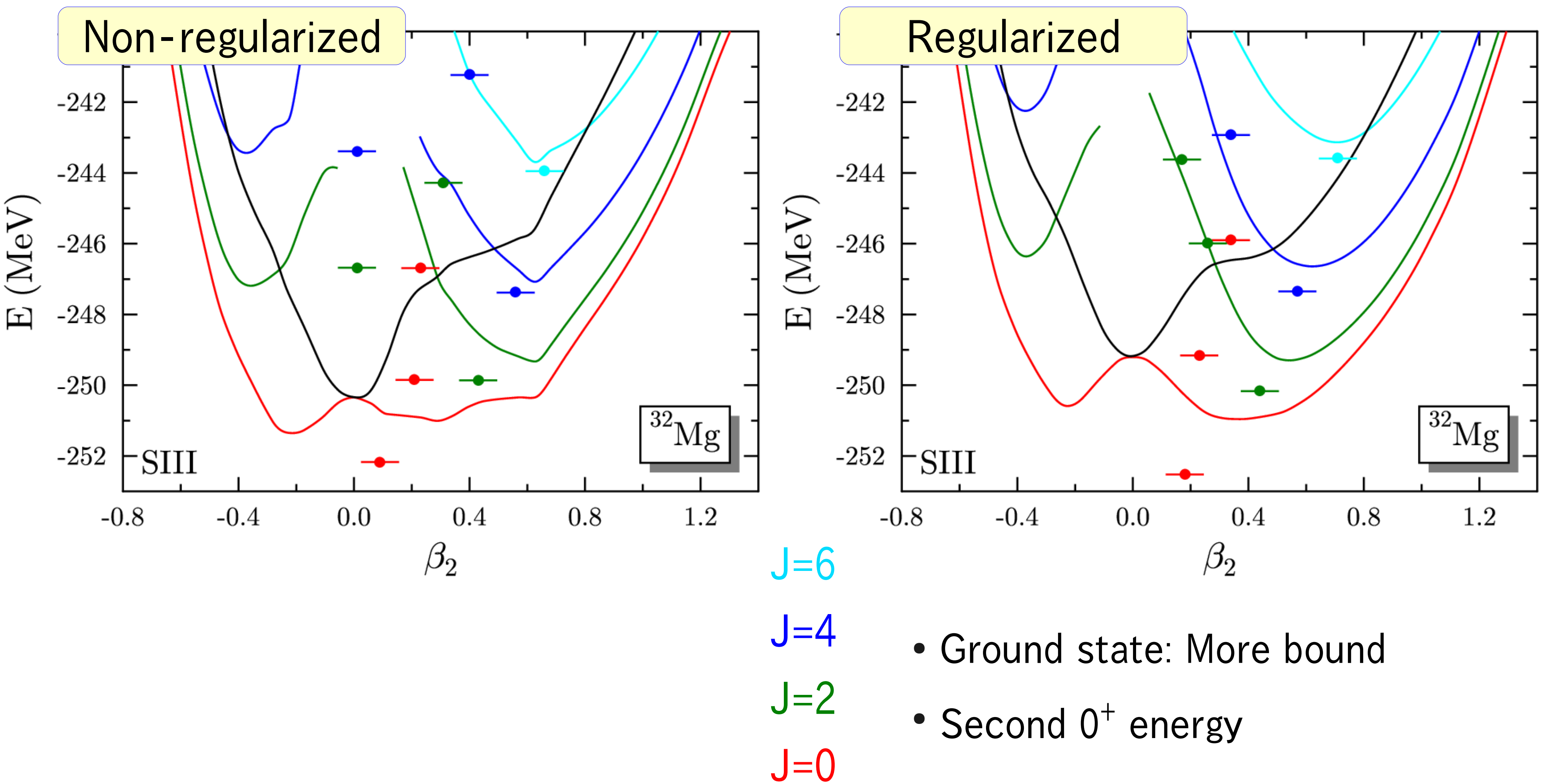
J=0

- SIII Skyrme interaction
- Volume type delta-pairing

  Pairing strength: 3 point formula of ^{30}Mg, ^{31}Mg, ^{32}Mg binding energies

Results

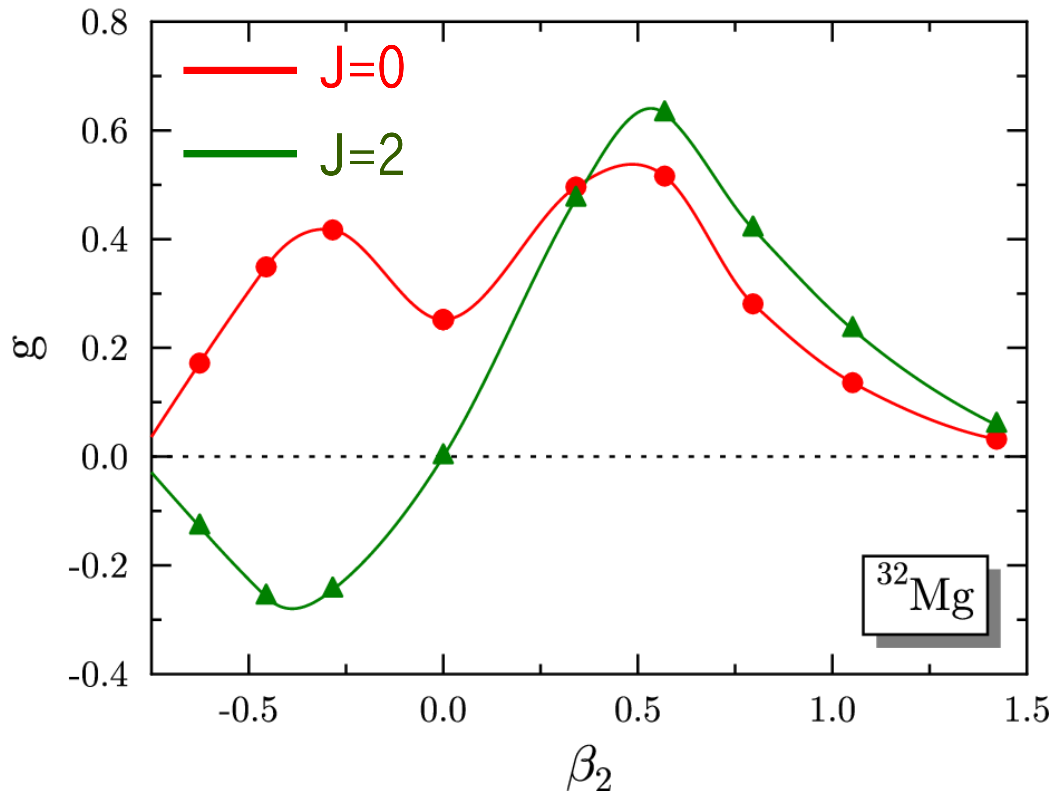
GCM collective energy

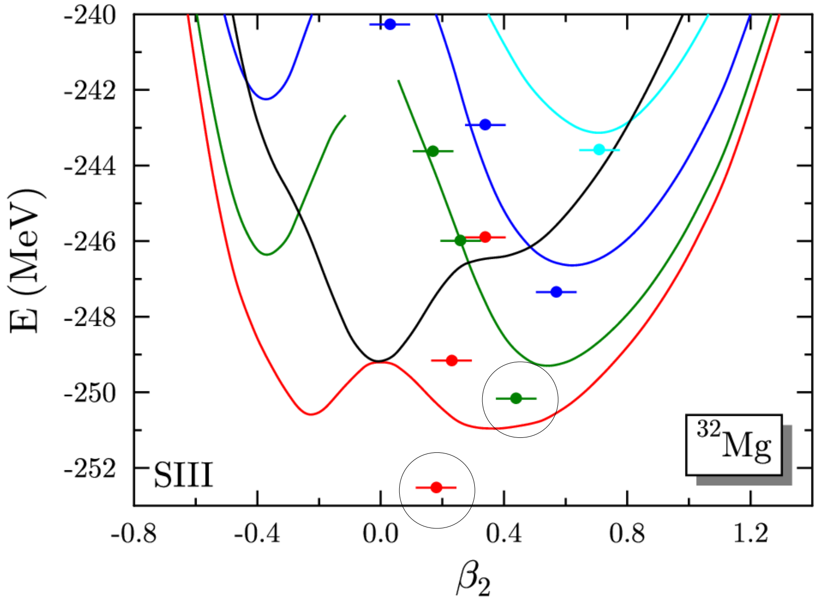


- Ground state: More bound
- Second 0^+ energy

Results

GCM collective wave function

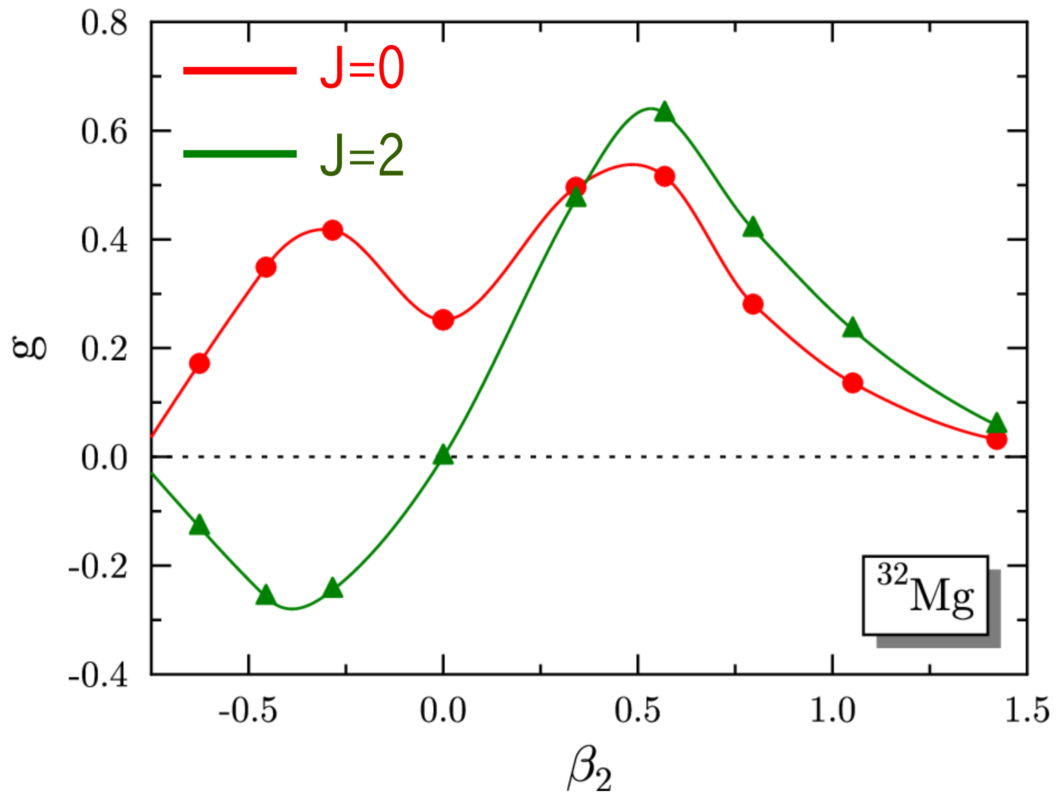


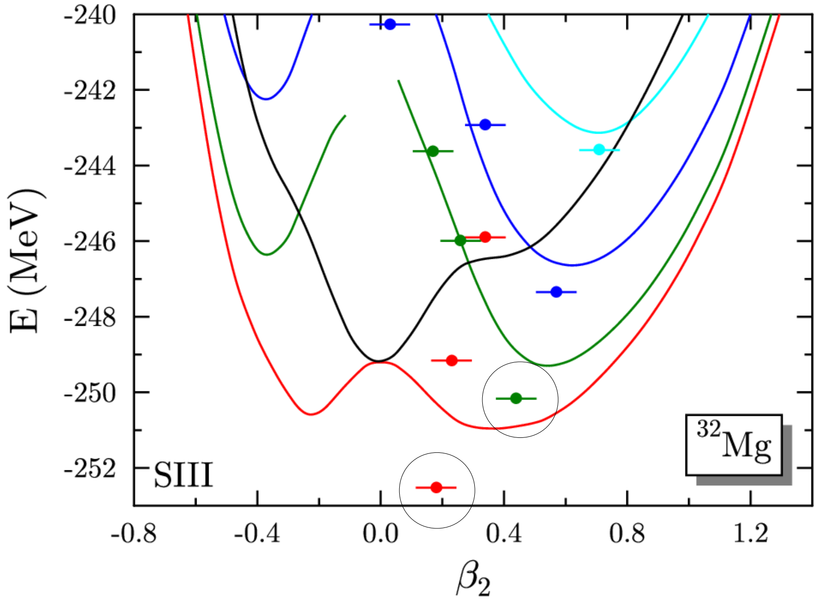


- Strong mixture of prolate and oblate states

Results

GCM collective wave function





- Strong mixture of prolate and oblate states

- Comparison with experimental data

	GCM	Exp. data
E_2 [MeV]	2.35	0.885
B(E2) [e^2 fm^4]	384	390±70

Summary & Outlook

- Configuration mixing calculations with regularization scheme
- Projected potential energy becomes smoother
- ^{32}Mg

  B(E2): good description

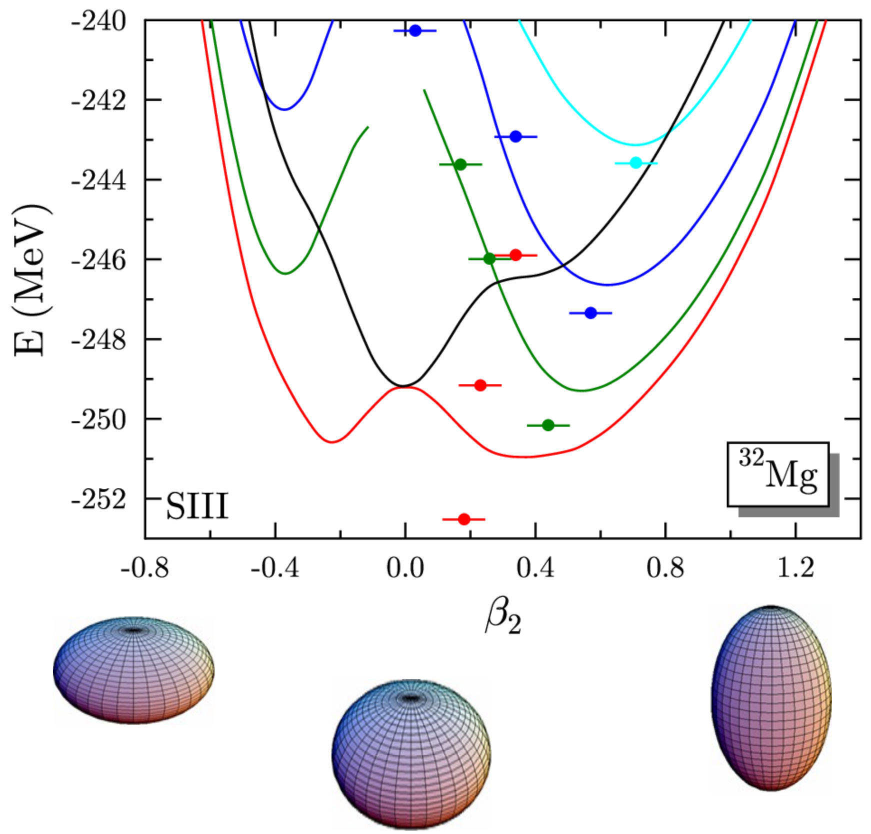
  E_2: overestimated

- SIII interaction adopted from old data

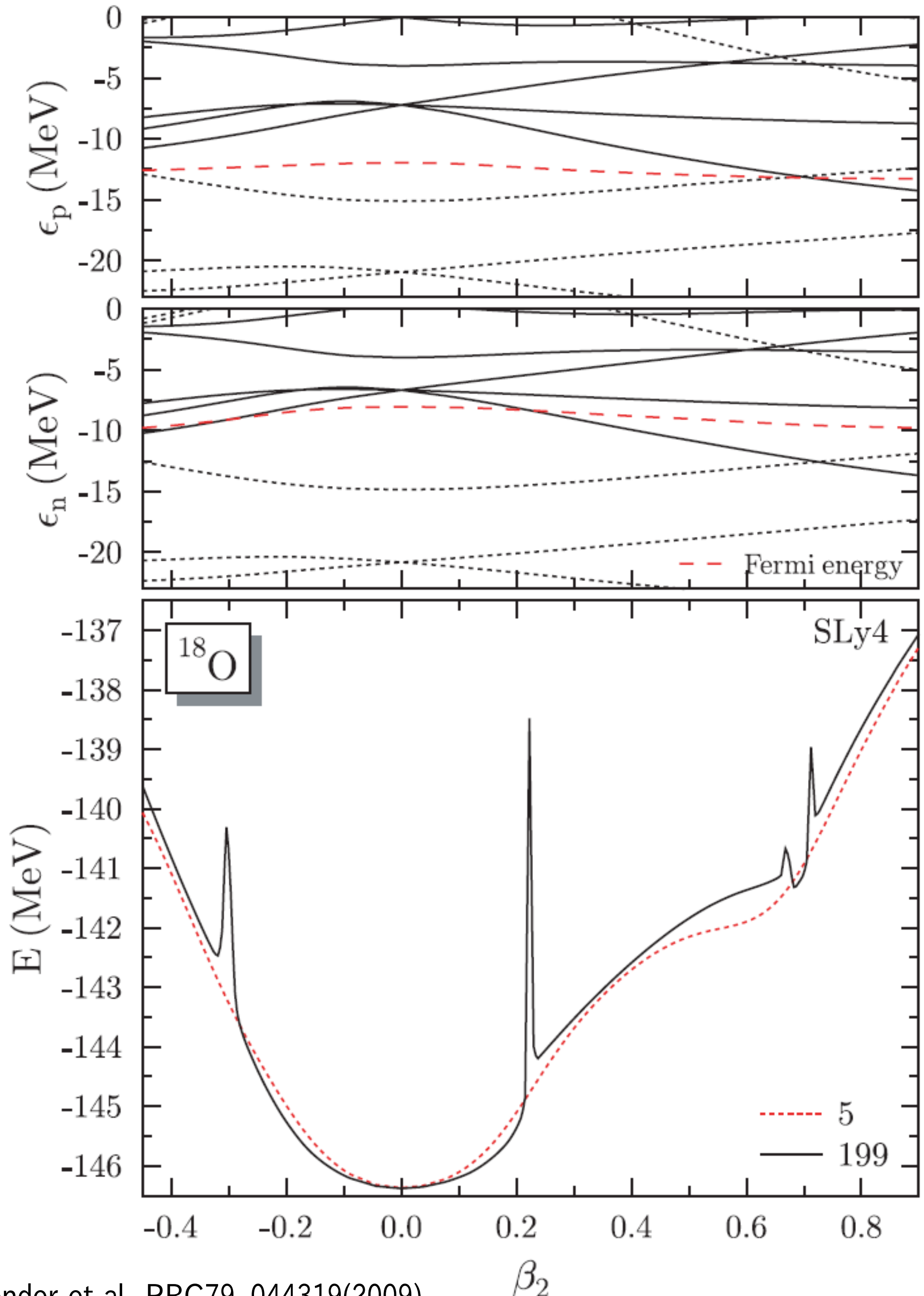
  → New effective interaction

- Structure of odd nuclei

  Configuration mixing of odd nuclei is in progress



Problems



Bender et al., PRC79, 044319(2009)

$$E(q) = \langle \Phi_N(q) | H | \Phi_N(q) \rangle$$

- Approximate use of functionals
  - Density-dependence
  - Different functionals between p-h and p-p channels

$$\langle \Phi | \Phi(\phi) \rangle = 0$$

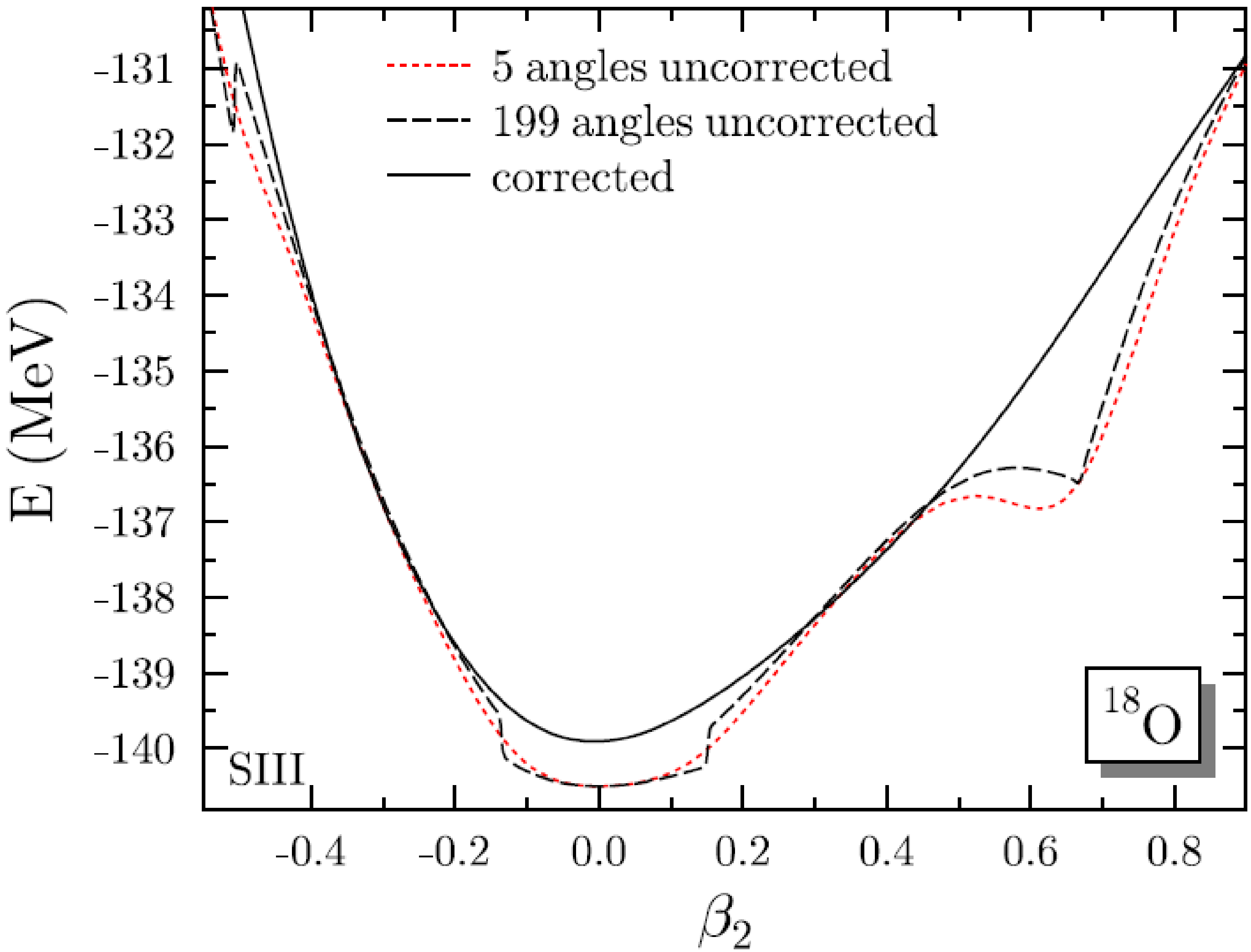
at $u_k^2 = v_k^2, \phi = \pi/2$

Anguiano et al., NPA696(2001)467

Lacroix et al., PRC79(2009)044318
Bender et al., PRC79(2009)044319
Duguet et al., PRC79(2009)044320

Regularization

Bender et al., PRC79, 044319(2009)



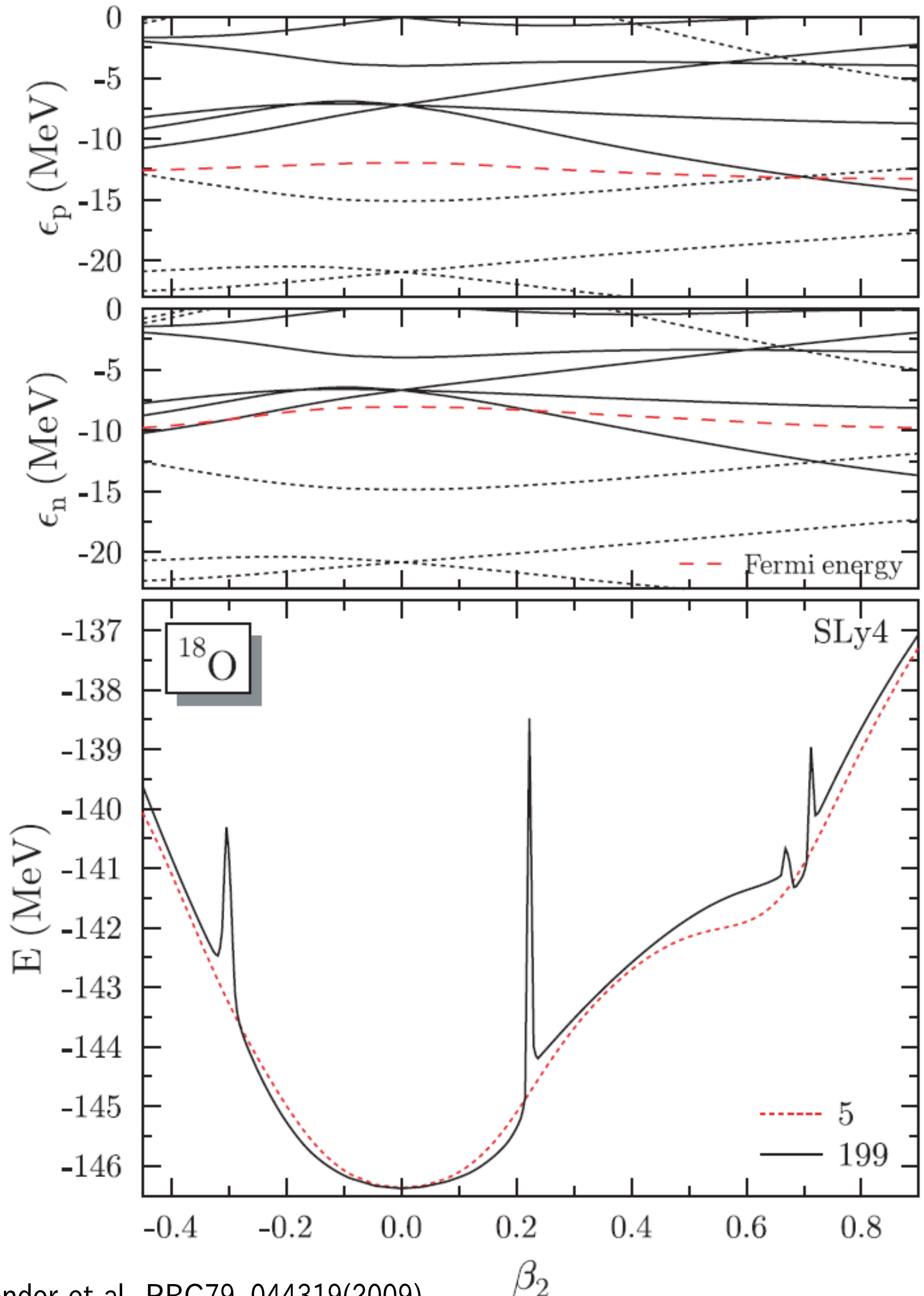
- Correction: a few MeV $\ll$ Total binding energy

  $\sim$ Excitation energy

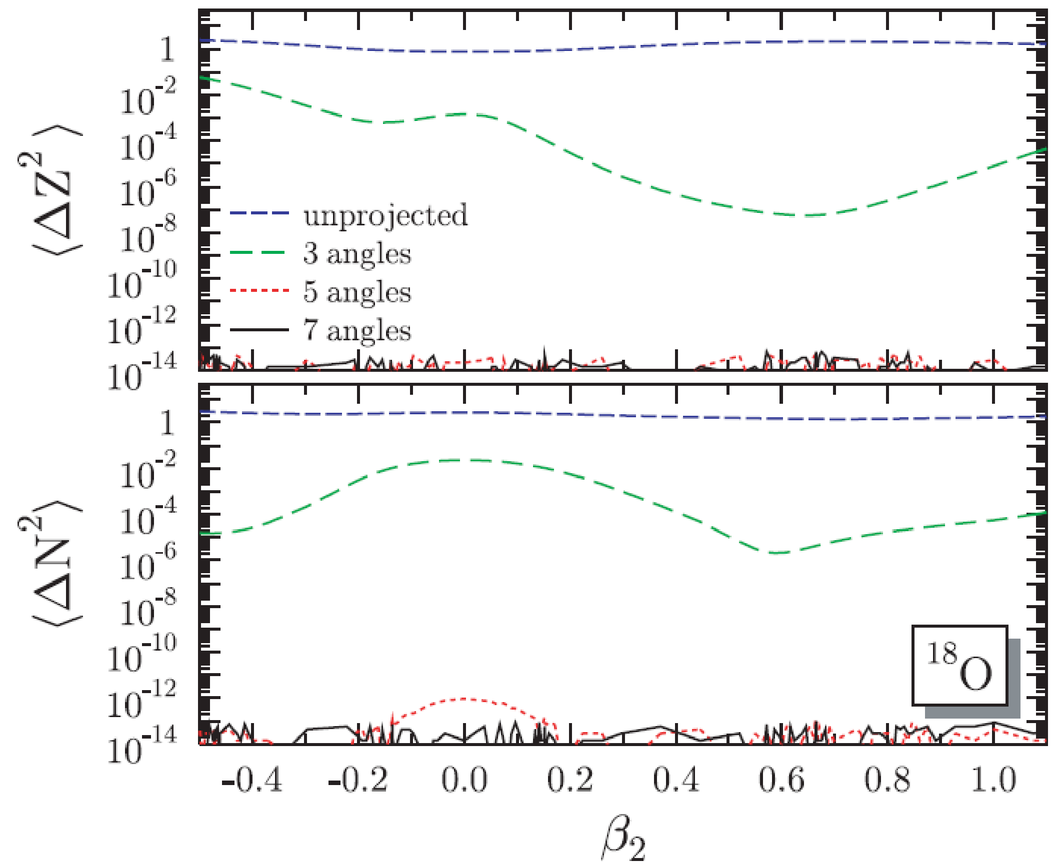
Skyrme energy density functional

$$
\begin{aligned}
\mathcal{H}_{\mathrm{Sky}}(\boldsymbol{r}) = {} & B_1\rho^2 + B_2(\rho_n^2 + \rho_p^2) \\
& + B_3(\rho\tau - \boldsymbol{j}^2) + B_4(\rho_n\tau_n - \boldsymbol{j}_n^2 + \rho_p\tau_p - \boldsymbol{j}_p^2) \\
& + B_5\rho\Delta\rho + B_6(\rho_n\Delta\rho_n + (\rho_p\Delta\rho_p) \\
& + B_7\rho^{2+\alpha} + B_8\rho^\alpha(\rho_n^2 + \rho_p^2) \\
& + B_9(\rho\nabla\cdot\boldsymbol{J} + \rho_n\nabla\cdot\boldsymbol{J}_n + \rho_p\nabla\cdot\boldsymbol{J}_p) \\
& + \cdots
\end{aligned}
$$

Problems



$$\langle \Delta \hat{N}^2 \rangle = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$$



Converged at L=5

Bender et al., PRC79, 044319(2009)

Regularization

Lacroix et al., PRC79(2009)044318
Bender et al., PRC79(2009)044319
Duguet et al., PRC79(2009)044320

- Divergence should be canceled out if $V_{ph} = V_{pp}$
  - ~~Use $V_{ph} = V_{pp}$~~
  - Regularization
    1. Pick up terms that would cancel out if $V_{ph} = V_{pp}$
    2. Remove these contribution from energy functionals

- Integer power of density-dependent terms in energy functionals

$$\mathcal{E}^{DD} = \int d^3r \left[B_7\rho^{2+\alpha} + B_8\rho^\alpha(\rho_n^2 + \rho_p^2)\right]$$

$\Rightarrow$ $\alpha \to 1$ $\Rightarrow$ SIII interaction

Beiner et al., NPA238(1975)29

c.f. SLy4, SkM*: $\alpha = 1/6$

Phenomenology of divergences in the PNP case

- Tajima et al, NPA542 (1992)
  - ➡ Early warnings
- Anguiano et al, NPA 696 (2001)
  - ➡ Divergences occur when a level crosses the Fermi energy, with occupation 0.5 and $\varphi = \pi/2$ at this point $\langle \Phi_0 | \Phi[\varphi] \rangle = 0$
  - ➡ The problem disappears if the same interaction (with exchange and coulomb treated properly) in the pp and ph channels.
  - ➡ First indication of the role of Generalized Wick Theorem (GWT)
- Dobaczewski et al, *PRC76 (2007)*
  - ➡ Analysis in the complex plane for the PNP case
- Bender and Duguet, Int.J. Mod. Phys. E16 (2007)
  - ➡ In the PNP case, by avoiding the use of GWT, one can cure the divergence problem even when different effective interaction are used in different channels.